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# Numerical analysis in field emission characteristics of carbon nanotube field emitters and arrays

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## Abstract

In this study, the field emission characteristics of carbon nanotube field emitters and arrays fabricated by carbon nanotube implantation process are analyzed by the combination of the finite-difference time-domain and particle-in-cell methods. Carbon nanotubes with different shapes are simulated and their electron trajectory properties are compared. A spacing optimized carbon nanotube field emission array is developed and the impact of random distribution in carbon nanotube length and tilt angle is also investigated. These results are useful to develop an optimized carbon nanotube field emission array that fits current fabrication capabilities.

**Keywords**
Carbon nanotube, field emission, finite difference time domain–particle-in-cell, random distribution array

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## Introduction

Since the identification of carbon nanotubes (CNTs) in 1991,[1] flourishing research into their properties has revealed many excellent characteristics, such as high aspect ratios, good conductivity and structural strength.[2–4] Currently CNTs are regarded as a promising candidate for vacuum microelectronic devices owing to their excellent field emission behaviors, including smart size, low threshold voltage, low power consumption and high emission current density.[5] CNTs have the potential of being used in field emission displays (FEDs),[6] X-ray tubes,[7] backlight units for liquid crystal displays,[8] and other cold-field emission devices, but micro fabrication processes must be improved before these expectations are realized.

The current density and beam convergence are two major evaluation factors for a good field emitter. The current density is determined by the Fowler–Nordheim equation.[9] The applied electric field and field enhancement factor are important parameters to determine emitted current; these are constrained by the shape and work function of nanotubes. Beam convergence is affected by emitting surface and electric field. The trajectory of electrons is the main indication of beam convergence. These parameters are important and need to be optimized during the actual CNT implantation process, but can hardly be observed in experiments. A numerical method is therefore introduced to simulate the field emission properties of a single nanotube and CNT arrays.

In this paper, the local field enhancement is studied in connection with different shapes of nanotubes (vertical and tilt aligned, rainbowed and spiral shaped) based on the CNT implantation process.[10] Further, the finite difference time domain (FDTD) method, combined with the particle-in-cell (PIC) method, is utilized to study the trajectory property of a certain emitter. The beam convergences of different shaped CNTs are compared. Meanwhile, a simple 2 μm × 2 μm field emission unit with 5 × 5 CNTs is analyzed. Current density and beam convergence of CNT arrays with random height and tilt angle distribution are analyzed compared with vertically aligned CNT arrays.

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## Numerical analysis methodologies

The electron trajectories of CNTs can scarcely be observed in experiments, so numerical methods are introduced for analyzing the field emission properties of CNT-based field emitters. In the numerical process, local field enhancement is studied on a single nanotube tip by examination of electric potential contours; in addition, the FDTD method is combined with the PIC method in a two-dimensional study of the relation between the CNT density and the current density for a certain emitter array.

Figure 1 shows the simulation process. The FDTD method is one of the basic methods in analysis of an electromagnetic field. It was implemented to solve the Maxwell equations in the emission domain with initial boundary conditions. In the initial calculation cycle, the electromagnetic fields on the meshed grids were calculated and stored. In order to demonstrate the trajectory of the electrons, the electric field between each calculated grid was numerically interpolated, and both momentum and position of the electron were evaluated according to the interpolated fields. By continuously evaluating the electron's velocity and position in $\Delta t$, we illustrate the trajectory process of the electron emitters. The trajectories were then used to determine the space charges of the emission electrons and set as conditions for evaluation of the electric field in iteration. The iteration stops if the deviation of space charge $|\Delta \vec{q}|$ is below $-10\,\text{dB}$.

The field emission current density is determined by Fowler–Nordheim equation[9]

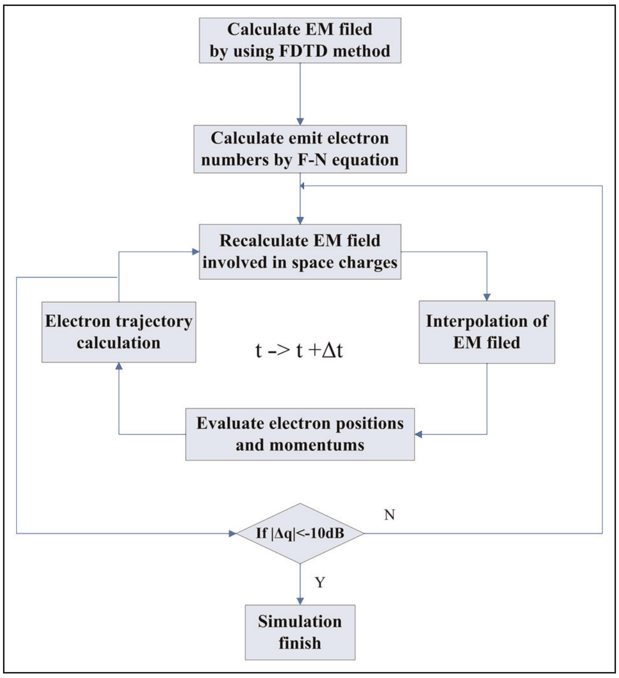

**Figure 1.** The simulation process of finite difference time domain–particle-in-cell method.

$$J = a\frac{F^2}{\varphi}\exp\left(-\frac{b\varphi^{\frac{3}{2}}}{F}\right) \tag{1}$$

In this equation, $F$ is the local electric field. $\varphi$ is the work function, which is typically 4.3–4.8 eV for multi-wall CNTs. We define $\varphi$ of the multi-walled CNTs as 4.8 eV. The parameters $a$ and $b$ are constants defined as

$$\begin{aligned} a &\equiv e^3/8\pi h_p = 1.84\times10^{-6}\ \ [\mathrm{AeVV^{-2}}] \\ b &\equiv \frac{8\pi}{3}(2me)^{1/2}/eh_p = 6.83\times10^{9}\ \ [\mathrm{VeV^{-3/2}m^{-1}}] \end{aligned} \tag{2}$$

The F-N function is used to calculate the current density on CNT surfaces in the electron trajectory simulation.

## Field enhancement and trajectory for different shapes of CNTs

Enhancement of the electric field takes place around the tips or protrusions of the nanotubes. The field enhancement factor is defined as the ratio of the applied field $E_{app}$ and the local field $E_{loc}$ as follows

$$\beta = E_{loc}/E_{app} \tag{3}$$

The CNT has a high aspect ratio $(10^2 - 10^3)$ and tip curvature(1–10 nm), which could enhance the local electric field and reduce the surface potential barrier markedly, so electrons can escape from the surface and form the field emission electrons. For a single CNT emitter, many parameters are responsible for its field emission property, such as aspect ratio, the anode–cathode distance, applied electric field and so on. Previous studies have shown that these parameters can influence the field emission properties.[11–13] During the actual CNT implantation process, however, the shapes and implanted patterns of CNTs are also important. As shown in Figure 2, the shapes of CNTs in an actual fabrication process are not always straight. This study mainly concerns the shape effect. Four common shapes of CNTs in actual fabrications are listed. A single CNT with the same length but different shapes – vertically aligned (Type a), tilt aligned (Type b), rainbowed (Type c) and spiral (Type d) – is investigated in Figure 3.

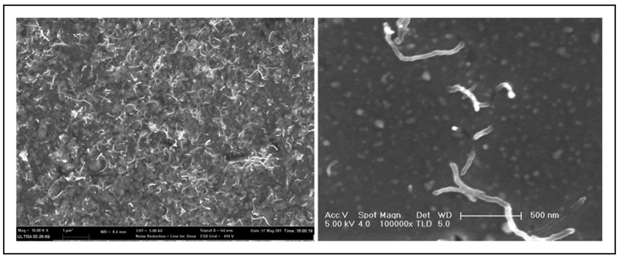

**Figure 2.** Scanning electron microscope images of the carbon nanotubes implanted on the electrode.

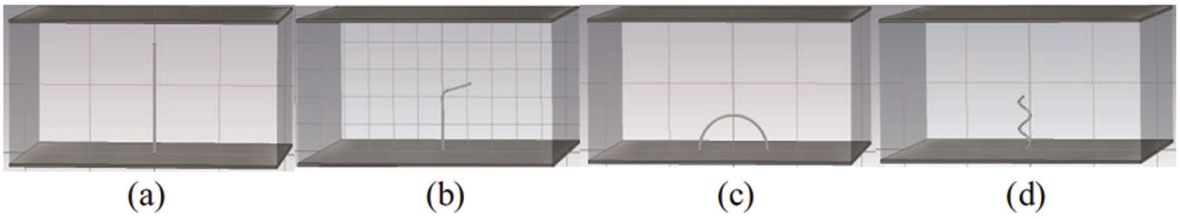

**Figure 3.** Scheme of different shaped single carbon nanotubes.

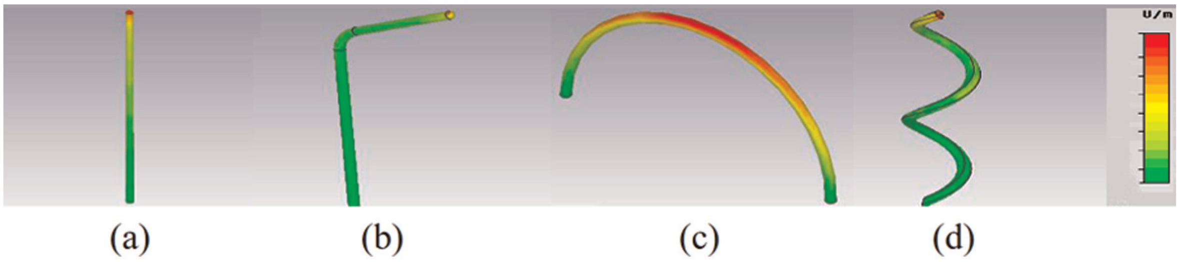

**Figure 4.** Electric field magnitude of different shaped carbon nanotubes.

In this study, a commonly used multi-walled CNT for which the mean nanotube's height is around 0.5 μm and radius around 5–20 nm is modeled. During numerical simulation, the single CNT is modeled as a cylinder 500 nm in height, with a radius of 10 nm. A simple field emission model was proposed by putting the CNT between two parallel electrodes with a distance of 1 μm. Boundary conditions were used to ground the cathode and the CNT and a 3V potential was applied on the anode; electric field magnitudes were best visualized using contour plots as in Figure 4.

The peak electric field magnitude can be found at CNT tips in Figure 4. As can be seen in Table 1, the peak E-field of a vertically aligned CNT is the maximum of the four, for which the field enhancement factor is 50.12. The tilted CNT is 45.50, the second largest, then the spiral and the rainbowed shaped CNTs. As the CNT is equipotential with the cathode, the electric potential of 90% of the CNT length on the bottom is relatively low; the electric field changed rmarkedly only around the tip. A CNT becomes more like a needle as its aspect ratio becomes larger, so the field enhancement effect is considerably more. The vertical shaped CNT has largest $\beta$ because it has the biggest equivalent aspect ratio. The enhancement factor for the tilted CNT is a little smaller as its equivalent aspect ratio decreases, while the trajectory area (the area for which local E-field is larger than $1 \times 10^8$ V/m) is far less than for the vertical CNT, as its tip is not facing the electric field direction. For the spiral CNT, the peak E-field can be found at its tip and curls, and for the rainbowed one, $\beta$ is the lowest because it does not have any sharp point or big inclination angle.

**Table 1.** Comparison of different shaped carbon nanotubes.

| Carbon nanotube shapes | Field enhancement factor | Divergence angle (rad) |
|---|---|---|
| Vertical | 50.12 | 0.128 |
| Tilt | 45.50 | 0.229 |
| Rainbowed | 12.80 | 0.286 |
| Spiral | 29.35 | 0.275 |

In Milne's work,[14] several CNT implantation methods were compared. The results showed that for CNTs produced by a commonly used method in industry, owing to its disorganized distribution and morphology, the field emission current density declines. For the numerical simulation results, Figure 5 shows a trajectory of beams and point clouds of beam spots on the anode. From Table 1 we c\n conclude that the vertically aligned CNT can reach the maximum field enhancement factor while at the same time having the best beam uniformity and convergency. The tilted CNT shows less convergence than the vertical one, and the other two are far worse.

## Field emission characteristics of CNT arrays

### *Optimization of CNT array spacing*

When the CNT field emission device was first introduced by de Heer,[6] only 0.1% of the total amount of CNTs were emitting electrons. This phenomenon is mainly attributed to the electrostatic screening effect, that is when the CNTs are close together, electrostatic

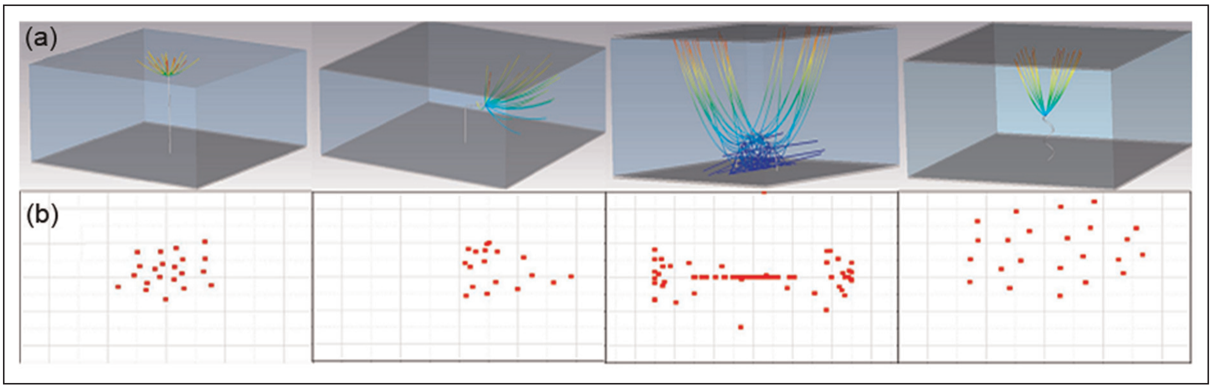

**Figure 5.** (a) Trajectory of beams of single carbon nanotube; (b) point clouds of beam spots on anode.

penetration would prevent the expected field enhancement. So during the fabrication of the CNT implanted electrode, controlling the spacing of the CNT array is meaningful. In this study, a simple 2 μm × 2 μm field emission unit with 5 × 5 vertically aligned, single CNT is optimized to the ideal spacing, which would guide the actual CNT implantation process.

Electrostatic screening has been clearly proved in simulation results. The simulation is of 2 μm × 2 μm field emission unit with CNT spacing 50 nm, 100 nm and 400 nm. Figure 6(b) shows a contour plot of E-field magnitude; from the CNT array shown in Figure 6(i) we could clearly see serious field penetration – there is a 60% reduction in E-field magnitude from marginal CNT to central CNT. For the CNT array with 100 nm spacing, the penetration has been noticeably weakened, and for the situation with 400 nm spacing, electrostatic screening has been perfectly eliminated. This has also been clarified by Figure 6(c). The peak electric field for CNT arrays with 400 nm spacing is near $2 \times 10^8$ V/m, for which the current density is in mA/cm$^2$. Many experiments have also proved that the intertube distance critically affects the field enhancement factor;[11,13,15] our simulation results accord well with the experiments and theoretical calculation. Owing to the enhanced screening of the electric field, the enhancement factor of the CNTs array decreases as the intertube distance is decreased; when the intertube distance was smaller than the nanotube height, the CNTs inside the array could not emit electrons.

## FE characteristics of CNT arrays with randomized height and orientation

Currently, the CNT implantation technique enables controllable CNT distribution density, strong mechanical adhesion between CNT and electrode, and the CNT distribution and exposition out of the electrode are also conducted in a random manner. As shown in Golovkoa's study,[14] CNTs are implanted using a highly purified cobalt colloid catalyst. This fabrication process can achieve a highly controllable CNT position, which can significantly enhance the field emission efficiency. As the CNTs were implanted into the electrode, the height and tilt angle of the exposed CNT array could also be varied. In this paper, two kinds of randomized distributed CNT arrays were simulated and compared with the vertically aligned CNT array to study the influence of the randomness in CNT height and tilt angle.

Figure 7(a), part (i) shows the scheme of the CNT array randomly distributed in height; in part (ii), we set the mean CNT height as 750 nm, and fluctuation range is 50 nm. E-field magnitude shown in part (iii) implies that the electric fields at each nanotube tip are not equal, but ranged from $1.29 \times 10^8$ V/m to $1.8 \times 10^8$ V/m. From Figure 7(b), we can discover that the point cloud on the anode is nearly uniformly distributed, but owing to the difference in height of the electron emitting position, the kinetic energy for electrons to reach the anode varies to a large extent, which may lead to reduction of the device life; meanwhile the orbits of electrons emitted from the lower tips may be affected by nearby CNTs, which may reduce the electron numbers reaching the anode. As can be confirmed from Table 2, serious fluctuations in height should be avoided.

During the process of CNT implantation, vertical alignment of the CNT is hard to obtain, so it is inevitable that CNT orientation deviates slightly from the E-field direction. In Figure 8(a), the random distribution in tilt direction is presented; we set the CNT tilt angle uniformly ranging from −30° to 30°, as can be seen in Figure 8(a), part (ii). From 8(a), part (iii), we discover that the electric field magnitude also declines, ranging from $1.01 \times 10^8$ V/m to $1.40 \times 10^8$ V/m. Also, the electron trajectory has been seriously affected – Figure 8(b) shows that more electrons do not collide on the anode, but fly away. This is because the velocity direction of the emitted electron is not along the E-field, owing to its tilt. Figure 8(b), part (ii) also implies that electron spots are not uniformly distributed. The emitting current density is 0.006 mA/mm$^2$ in Table 2, which is a great reduction compared to the vertically aligned CNT arrays.

Compared with the formal experiment results,[16–18] our modeling CNT density is 6.25/μm$^2$, and the applied

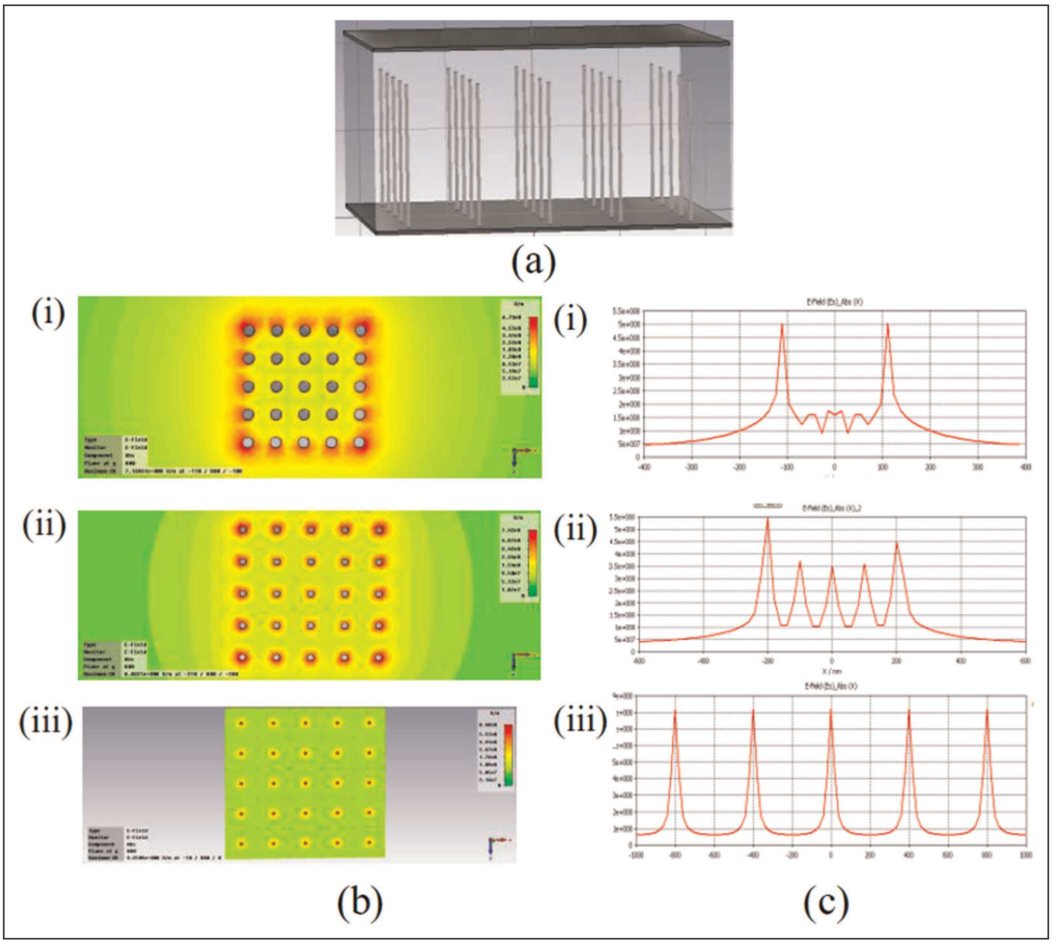

**Figure 6.** (a) Scheme of carbon nanotube array; (b) contour plot of electric field magnitude on tip surface; (c) electric field magnitude on axis.

**Table 2.** Field emission characteristics of different types of carbon nanotube arrays.

| Array types | Current density (mA/mm$^2$) | Emitted electron numbers | Electrons colliding on anode |
|---|---|---|---|
| Vertical aligned | 6.97 | 525 | 476 |
| Random height | 0.592 | 525 | 458 |
| Random orientation | 0.006 | 496 | 160 |

electric field is 3 V/μm, which is within the range of the common fabricated CNT emitter cells (5–8/μm$^2$, 1–5 V/μm),[16] and for the experimental results, the current density ranges from 10 mA/cm$^2$ to 100 mA/cm$^2$. The simulation shows consistency with the experiment, and indicates that high equivalent aspect ratio is important to improve CNT field emission properties. During the implantation process, a large tilt angle should be avoided.

## Summary

The field emission characteristics of CNT field emitters produced using a CNT implantation process were analyzed using the FDTD and PIC method. The vertically aligned single CNT has the maximum field enhancement factor, compared to CNTs with equal length but other attitudes. The vertically aligned single CNT is also proved to be best of the four CNT shapes in terms of convergence and uniformity of the trajectory beams.

For the CNT field emission arrays, the simulation result shows that single nanotube spacing should not be too small, as the electrostatic screening effect would prevent the expected field enhancement. Compared to the ideal equal length, vertically aligned CNT array, CNT arrays with randomized length and tilt angle distribution have drawbacks, such as decreased current density and weakened electron trajectory characters. The simulation result implies that in the fabrication process of the CNT field emission unit, large fluctuations of CNT length and tilt should be avoided.

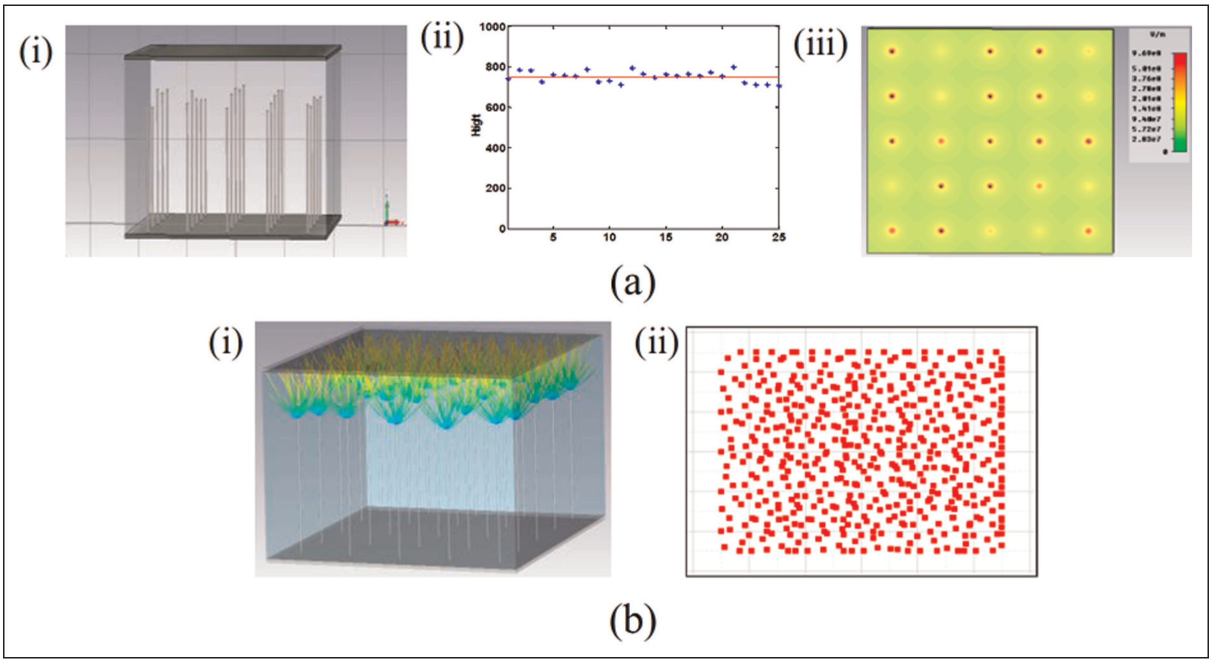

**Figure 7.** (a), Part (i) scheme of a carbon nanotube array with randomized length; part (ii) carbon nanotube length distribution; part (iii) contour plot of electric field magnitude on surface (z = 750 nm); (b), part (i) trajectory of beams of carbon nanotube array; part (ii) point clouds of beam spots on anode.

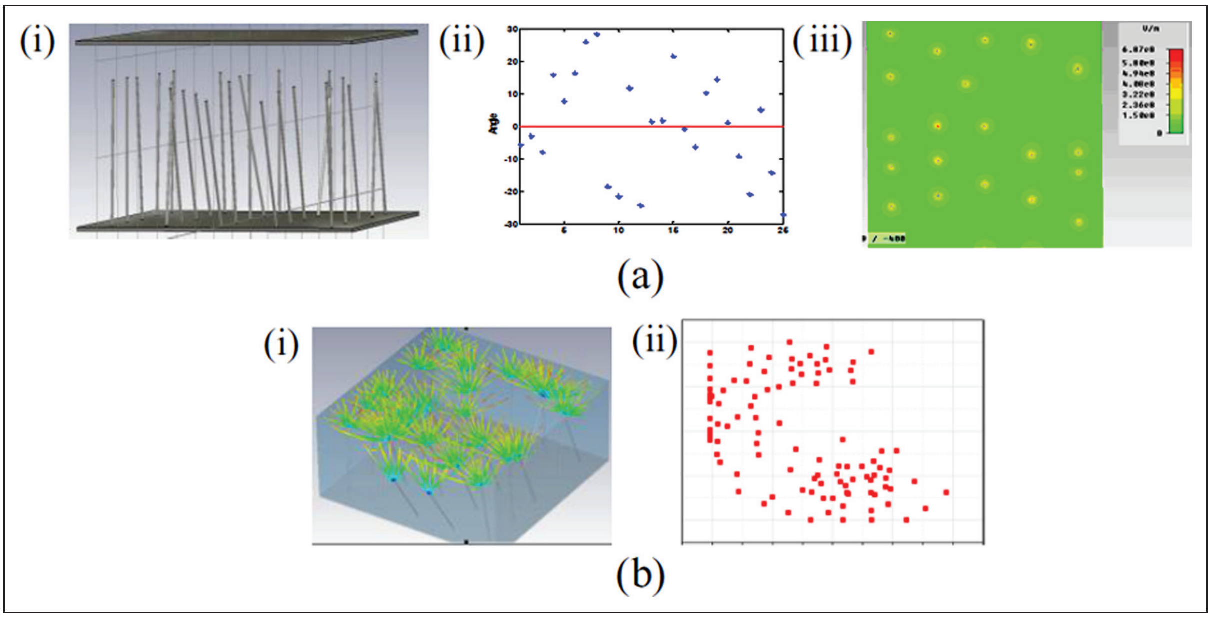

**Figure 8.** (a), Part (i) scheme of a carbon nanotube array with randomized orientation; part (ii) carbon nanotube tilt angle distribution; part (iii) contour plot of electric field magnitude on surface (z = 750 nm); (b), part (i) trajectory of beams of carbon nanotube array; part (ii) point clouds of beam spots on anode.

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